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A THREE-PHASE FINITE ELEMENT MODEL OF WATER-INFILTRATED POROUS MATERIALS SUBJECTED TO FREEZING

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Abstract. In areas of geotechnical engineering, artificial ground freezing is commonly used as an effective way to deal with various ground construction challenges such as groundwater control and temporary excavation support. For the description of the coupled thermo-hydro-mechanical behavior of soil exposed to frost action, this paper presents a three-phase Finite Element model of porous materials, consisting of solid skeleton, liquid water and crystal ice, where the liquid phase contains both weakly-bound pore water and strongly-bound water film. Within the theory of thermo-poroelasticity proposed by Coussy [1, 2], poroelastic constitutive relations are provided from an energy approach of poromechanics. In addition, the phase transition between water and ice is characterized by a purely temperature-dependent thermodynamic state function named liquid saturation degree considering the pore size distribution. The cryo-suction mechanism that induces migration of water towards the frozen sites is impelled by the chemical potential difference existing between the pre-melted water film and the adjacent pore water. By choosing solid displacement, liquid pressure and mixture temperature as principal unknowns, the model is implemented in a geometrically-linear Finite Element context base upon the governing balance equations for the soil constituents and their mixture. The validation procedure is shown by selected examples with analyses of different aspects of the model behavior.

1 INTRODUCTION

Freezing of porous materials is of great interest to a wide range of fields such as geotechnical engineering, food industry, environmental engineering and biomechanics. In areas of geotechnical engineering, artificial ground freezing, which can be achieved by using either a large portable refrigeration plant or liquid nitrogen, is often used as an effective ground improvement technique to deal with various geotechnical construction challenges such as groundwater control and temporary excavation support. Yet, the potential problem of this technique is that it may produce frost heave and thaw settlement at the ground surface, which have deleterious consequences among surface infrastructure. Moreover, the closure of the frozen-soil body is significantly influenced by the groundwater flow especially when the seepage velocities are high. Consequently, for the sake of a safe design and execution, such applications require a correct prediction of the coupled thermo-hydro-mechanical behavior of porous materials upon freezing.

However, the mechanics of porous materials subjected to frost action is way more complex than simply that of a sealed water-filled bottle, since porous solids with pores of various sizes behave intriguing and even counterintuitive. A well-known interpretation is the unexpected expansion observed during the freezing of a sealed cement paste sample filled up with benzene, which contracts when solidifying [3]. During freezing, fully coupled thermo-hydro-mechanical processes are generally involved such as phase transition between constituents as well as the cryo-suction mechanism driving the liquid towards the frozen sites. Recent works have been devoted to the modeling of the behavior of porous materials exposed to freezing. A mathematical freezing model for saturated soil has been established by Mikkola & Hartikainen [4, 5, 6] based on the mixture theory and basic principles of thermomechanics. Similarly, a three-phase freezing model of saturated porous media (solid, pore fluid and pore ice) has been developed by Bluhm et al. [7, 8] within the framework of Theory of Porous Media (Boer [9] and Ehlers [10]). Nevertheless, both models provide little physical explanation for the observed phenomena such as the cryo-suction process that sucks liquid water towards the already frozen sites. Coussy has proposed a comprehensive thermo-poroelastic theory for the description of mechanical behavior of water-infiltrated materials upon freezing [1, 2, 11, 12], which specifies the multi-scale physics of confined crystallization of ice and provides more physics-based understanding by means of exploring how the macroscopic properties can be upscaled from the knowledge of microscopic properties. Thereby, as a result of careful evaluation, the theory of thermo-poroelasticity proposed by Coussy is adopted as the basis for present research.

Based upon the adopted theory, a three-phase Finite Element model of porous materials, consisting of solid skeleton, liquid water and crystal ice, is present in this paper to describe the behavior of water-infiltrated materials upon freezing. The setting up of the liquid-crystal thermodynamic equilibrium provides a relation between the crystal pressure and liquid pressure, which in the sequel plays an important role on the cryo-suction mech-

anism. The phase transition between water and ice is incorporated via a temperature-dependent liquid saturation function characterized by pore size distribution. Poroelastic constitutive relations are obtained from an energy approach of poromechanics. Stemming from the governing balance equations, the coupled set of differential equations for solid displacement, liquid pressure and mixture temperature is formulated in a geometrically-linear Finite Element context and implemented in an object-oriented Finite Element code (KRATOS). The validity of the model is demonstrated by three selected examples with analyses of the main characteristics of the behavior of freezing porous materials.

2 MODELING OF FREEZING POROUS MATERIALS

According to the adopted poromechanics theory [1, 2], the behavior of freezing porous materials can be essentially described at the macroscopic scale by the following set of equations: (1) liquid-crystal equilibrium relation, (2) liquid saturation curve, and (3) constitutive equations.

2.1 The liquid-crystal equilibrium relation

Thermodynamic equilibrium between the liquid pore water (L) and the adjacent crystal ice (C) requires the equality of the chemical potential of both phases

$$\mathrm{d}\mu_{\mathrm{L}} = \mathrm{d}\mu_{\mathrm{C}}\,, \quad \text{with} \quad \mathrm{d}\mu_{\mathrm{J}} = \frac{\mathrm{d}\,p_{\mathrm{J}}}{\rho_{\mathrm{J}}} - s_{\mathrm{J}}\,\mathrm{d}\,T \quad (\mathrm{J}=\mathrm{L},\mathrm{C})\,, \tag{1}$$

where p_{J}, ρ_{J} and s_{J} are the pressure, the specific mass density and the entropy per unit mass of phase J, respectively. Integrating the above equation between the reference state ($p = 0\,\mathrm{Pa}$, $T = T_{\mathrm{f}} = 273\,\mathrm{K}$) and the current state provides the liquid-crystal equilibrium condition

$$p_{\mathrm{C}} - p_{\mathrm{L}} = \Sigma_{\mathrm{f}}\,(T_{\mathrm{f}} - T)\,, \quad \text{with} \quad \Sigma_{\mathrm{f}} = \frac{\rho_{\mathrm{C}} L_{\mathrm{f}}}{T_{\mathrm{f}}}\,, \tag{2}$$

where T_{f}, Σ_{f} and L_{f} are the freezing temperature, the freezing entropy and the latent heat of freezing, respectively.

2.2 The liquid saturation curve

The mechanical equilibrium of the liquid-crystal interface is governed by the YOUNG-LAPLACE law

$$p_{\mathrm{C}} - p_{\mathrm{L}} = \frac{2\,\gamma_{\mathrm{CL}}}{R}\,, \tag{3}$$

where γ_{CL} is the liquid-crystal interface energy and R is the mean curvature radius of the interface. If a zero contact angle between the liquid and the solid skeleton is assumed for simplicity, R denotes also the pore radius where the current liquid-crystal interface locates. Combining Eqs. (2) and (3) yields the GIBBS-THOMSON relation

$$R = \frac{2\,\gamma_{\mathrm{CL}}}{\Sigma_{\mathrm{f}}\,(T_{\mathrm{f}} - T)}\,, \tag{4}$$

which implies that all the pores having an entry radius greater than R will freeze at the given temperature T, and the remaining ones being filled with liquid water. This allows us to retrieve the existence of a state relation linking the liquid saturation and the temperature.

The determination of this relation can be inferred from the knowledge of the capillary curve, which relates the liquid saturation to the capillary pressure. For a porous material partially saturated by liquid water, and whose remaining porous space is filled by air (G), the capillary curve can be described by the function of VAN GENUCHTEN [13]

$$p_{\mathrm{G}} - p_{\mathrm{L}} = \mathcal{N}({S_{\mathrm{L}}}^{-\frac{1}{m}} - 1)^{1-m}\,, \quad 0 < m < 1\,, \tag{5}$$

where p_{G}, $\mathcal{N}$ and m are the gas pressure, the capillary modulus and a constant representing the shape of the capillary curve, respectively. Similarly to Eq. (3), the YOUNG-LAPLACE law at the gas-liquid interface reads

$$p_{\mathrm{G}} - p_{\mathrm{L}} = \frac{2\,\gamma_{\mathrm{GL}}}{R}\,, \tag{6}$$

where γ_{GL} is the liquid-air interface energy. Combination of Eqs. (5) and (6) provides a relationship between the liquid saturation and the pore size

$$S_{\mathrm{L}} = \left(1 + \left(\frac{2\,\gamma_{\mathrm{GL}}}{\mathcal{N}\,R}\right)^{\frac{1}{1-m}}\right)^{-m} = S(R)\,, \tag{7}$$

which denotes that the remaining liquid saturation S_{L} equals to the cumulative fraction $S(R)$ of pore volume occupied by pores having a pore entry smaller than R, according to the standard mercury porosimetry [14, 12].

Replacing the pore size R in (7) by the GIBBS-THOMSON law (4) gives a relationship between the liquid saturation and the temperature

$$S_{\mathrm{L}} = \left(1 + \left(\frac{\Delta T}{\Delta T_{\mathrm{ch}}}\right)^{\frac{1}{1-m}}\right)^{-m}\,, \tag{8}$$

where $\Delta T = T_{\mathrm{f}} - T$ is defined as the current cooling and $\Delta T_{\mathrm{ch}} = \frac{\mathcal{N}\,\gamma_{\mathrm{CL}}}{\Sigma_{\mathrm{f}}\,\gamma_{\mathrm{GL}}}$ the characteristic cooling. The parameters ΔT_{ch} and m are closely related to the pore size and pore size distribution (cf. Boukpeti [15]). Their influences on the shape of the saturation curve are illustrated in Fig. 1.

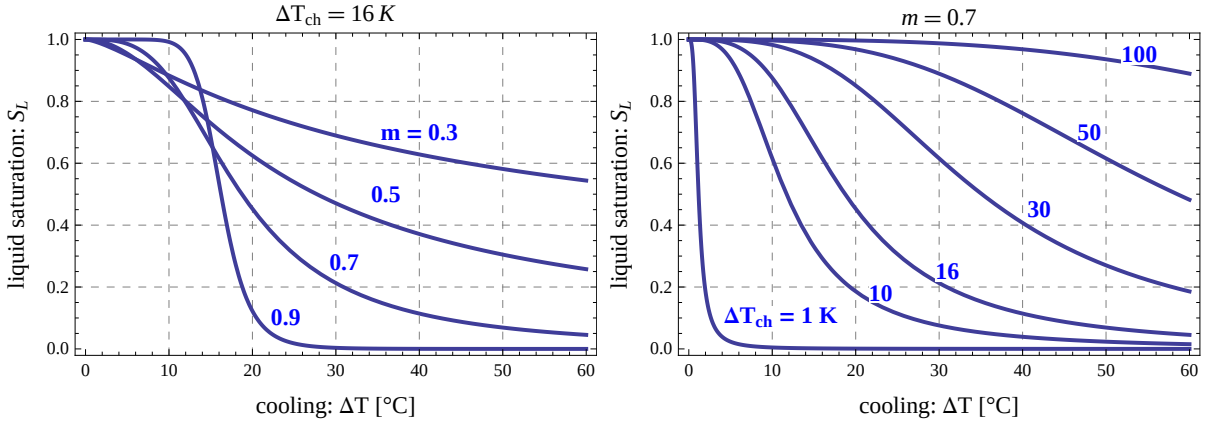

Figure 1: Liquid saturation curve during freezing by influences of m (left) and ΔT_{ch} (right).

2.3 Constitutive equations

To describe the mechanical behavior of freezing porous materials, the thermo-poroelastic constitutive equations, developed by Coussy [2] using an energy approach, are adopted. Consider a representative volume $\mathrm{d}\,\Omega_0$ extracted from a partially frozen porous material with an initial porosity ϕ_0, an initial temperature T_0 and a (zero) reference pore pressure of atmospheric pressure. The current (Lagrangian) porosity ϕ can be written as

$$\phi = \phi_{\mathrm{L}} + \phi_{\mathrm{C}}\,, \quad \phi_{\mathrm{J}} = \phi_0\, S_{\mathrm{J}} + \varphi_{\mathrm{J}}\,, \tag{9}$$

where ϕ_{J} is current partial porosity occupied by phase J, φ_{J} the respective change in partial porosity, and S_{J} the respective current saturation with $S_{\mathrm{L}} + S_{\mathrm{C}} = 1$. Recalling the standard micro-macro relations [1] and assuming that all pores deform the same when subjected to the same pore pressure, the total stress tensor $\boldsymbol{\sigma}$ and the partial porosity change φ_{J} are related to the strain tensor $\boldsymbol{\varepsilon}$, the pore pressures p_{J} and the temperature T as following

$$\begin{aligned}
\sigma_{ij} &= (K - \tfrac{2}{3}\,G)\,\epsilon\,\delta_{ij} + 2\,G\,\varepsilon_{ij} - b\,(S_{\mathrm{L}}\,p_{\mathrm{L}} + S_{\mathrm{C}}\,p_{\mathrm{C}})\,\delta_{ij} - 3\,\alpha_{\mathrm{S}}\,K\,(T - T_0)\,\delta_{ij}\,; \\
\varphi_{\mathrm{L}} &= b\,\epsilon\,S_{\mathrm{L}} + \frac{p_{\mathrm{L}}}{N_{\mathrm{LL}}} + \frac{p_{\mathrm{C}}}{N_{\mathrm{CL}}} - \alpha_{\mathrm{S}}\,(b - \phi_0)\,(T - T_0)\,S_{\mathrm{L}}\,; \\
\varphi_{\mathrm{C}} &= b\,\epsilon\,S_{\mathrm{C}} + \frac{p_{\mathrm{L}}}{N_{\mathrm{CL}}} + \frac{p_{\mathrm{C}}}{N_{\mathrm{CC}}} - \alpha_{\mathrm{S}}\,(b - \phi_0)\,(T - T_0)\,S_{\mathrm{C}}\,,
\end{aligned} \tag{10}$$

where $\epsilon = \varepsilon_{kk}$ is the volumetric dilation; K and G are respectively the bulk modulus and the shear modulus of the solid skeleton subjected to condition $p_{\mathrm{L}} = p_{\mathrm{C}} = 0$; k_{S} and α_{S} are respectively the bulk modulus and the linear thermal dilation coefficient of the solid matrix, that is the solid part of the porous solid; while b and N_{JK} are respectively the Biot coefficient related to the solid skeleton and the generalized Biot coupling moduli satisfying the Maxwell symmetry relation $N_{\mathrm{CL}} = N_{\mathrm{LC}}$ and $\frac{1}{N_{\mathrm{JJ}}} + \frac{1}{N_{\mathrm{LC}}} = \frac{b-\phi_0}{k_{\mathrm{S}}}\,S_{\mathrm{J}}$. Hence, the current porosity yields

$$\phi = \phi_0 + b\,\epsilon + \frac{b-\phi_0}{k_\mathrm{S}}\left(S_\mathrm{L}\,p_\mathrm{L} + S_\mathrm{C}\,p_\mathrm{C}\right) - \alpha_\mathrm{S}\,(b-\phi_0)\,(T-T_0)\,. \tag{11}$$

It is worthwhile to note that if the approximation $\varphi_\mathrm{J} \approx (\varphi_\mathrm{L} + \varphi_\mathrm{C})\,S_\mathrm{J}$ is made, the current partial porosities can be obtained via $\phi_\mathrm{J} = \phi\,S_\mathrm{J}$.

3 GOVERNING BALANCE EQUATIONS

With the above formulation of the constitutive relations, adopting linearized geometrical relations, the problem of a freezing water-infiltrated porous material exposed to freezing temperatures is described by the governing balance equations, which form the set of differential equations to be solved by the Finite Element Method (FEM). In the present work, the model development was restricted to isotropic thermo-poroelasticity under the assumption of small deformations. For the formulation of the balance equations it is assumed that the pore volume is at all time fully-saturated – partly occupied by ice crystals and partly occupied by the water remaining in liquid form. By choosing the displacement $\mathbf{u}$, the liquid water pressure p_L and the mixture temperature T as primary variables, the set of field equations was derived as summarized below.

3.1 Mass balance of liquid water and crystal ice

Taking into account the possible phase transition between liquid water and crystal ice, the mass balance equation relative to each phase can be written as

$$\frac{\mathrm{d}\,m_\mathrm{L}}{\mathrm{d}\,t} + \nabla\cdot\mathbf{w}_\mathrm{L} = -\overset{\circ}{m}_{\mathrm{L}\to\mathrm{C}}\,, \quad \frac{\mathrm{d}\,m_\mathrm{C}}{\mathrm{d}\,t} + \nabla\cdot\mathbf{w}_\mathrm{C} = \overset{\circ}{m}_{\mathrm{L}\to\mathrm{C}}\,, \tag{12}$$

where $m_\mathrm{J} = \rho_\mathrm{J}\,\phi_\mathrm{J}$ stands for the current mass content related to phase J per unit of initial volume $\mathrm{d}\,\Omega_0$, while $\overset{\circ}{m}_{\mathrm{L}\to\mathrm{C}}$ is the rate of liquid water mass changing into crystal ice per $\mathrm{d}\,\Omega_0$. Normally, the ice flow is slow, so that $\mathbf{w}_\mathrm{C} = \mathbf{0}$ can be assumed. Summation of these two equations yields the mass balance for the liquid water and the crystal ice

$$\frac{\mathrm{d}\,m_\mathrm{L}}{\mathrm{d}\,t} + \frac{\mathrm{d}\,m_\mathrm{C}}{\mathrm{d}\,t} + \nabla\cdot\mathbf{w}_\mathrm{L} = 0. \tag{13}$$

In addition the liquid water flow $\mathbf{w}_\mathrm{L}$ is assumed to be governed by Darcy's law.

3.2 Overall momentum balance

Disregarding dynamic effects, the momentum balance equation for the mixture is given as:

$$\nabla\cdot\boldsymbol{\sigma} + \rho\,\mathbf{g} = 0\,, \tag{14}$$

where ρ stands for the overall mass density of the porous material and $\mathbf{g}$ for the gravity forces per unit volume.

3.3 Overall entropy balance

Under the assumption of small perturbations, small variations of the temperature, the entropy balance for the mixture can be derived as:

$$T\left(\frac{\mathrm{d}\,\Sigma_{\mathrm{S}}}{\mathrm{d}\,t}+m_{\mathrm{L}}\frac{\mathrm{d}\,s_{\mathrm{L}}}{\mathrm{d}\,t}+m_{\mathrm{C}}\frac{\mathrm{d}\,s_{\mathrm{C}}}{\mathrm{d}\,t}+(s_{\mathrm{C}}-s_{\mathrm{L}})\,\frac{\mathrm{d}\,m_{\mathrm{C}}}{\mathrm{d}\,t}\right)+\nabla\cdot\mathbf{q}=0\,, \tag{15}$$

where $\Sigma=\Sigma_{\mathrm{S}}+m_{\mathrm{L}}\,s_{\mathrm{L}}+m_{\mathrm{C}}\,s_{\mathrm{C}}$ is the overall density of entropy per unit of volume, while Σ_{S} is the entropy of the solid matrix, s_{J} the specific entropy related to liquid water or crystal ice, and $\mathbf{q}$ the outgoing heat flow vector. Considering isotropy, FOURIER's law is given as $\mathbf{q}=-k\nabla T$, where k is the thermal conductivity.

4 FINITE ELEMENT FORMULATION

In the context of the Finite Element formulation of the model in a geometrically linear setting, the balance equations (13)-(15) are transformed to their variational forms. For the spatial discretization of the initial boundary value problem, quadratic Lagrangian shape functions are used for the approximation of the displacement field and linear shape functions are used for the approximations of the liquid pressure and the temperature. With such approximations the BABUSKA-BREZZI stability constraint is fulfilled [16]. For the temporal discretization, a modified midpoint rule, denoted as the generalized-α method is used, which ensures unconditional stability and second order accuracy for an appropriate choice of its parameters [17]. The discretized weak form, evaluated at the generalized midpoint, yields a highly nonlinear system of equations that is solved iteratively using NEWTON's method. For the sake of simplicity, the tangent stiffness matrices required to solve the linearized system of algebraic equations are generated numerically according to the methodology presented by Lee & Park [18]. Finally, the three-phase freezing model for saturated soils has been implemented into the object-oriented FE-code KRATOS (Dadvand et al.[19]).

5 MODEL VALIDATION

Once the numerical model has been established, a validation procedure has been initiated in order to demonstrate, that the proposed formulation can be used to reproduce the main characteristics of the behavior of freezing porous materials. The adopted validation strategy is characterized by three steps, in which different aspects of the model behavior are analyzed.

5.1 Phase transition with latent heat effect

The model performance with regards to the phase change behavior and the latent heat effect of freezing soils is first investigated by comparing the numerical results with the phase-change model presented by Lackner et al. [20], where only the thermal problem is

considered. A cuboid fully saturated sand specimen with a height of 0.09 m and a cross-section of 0.41 m by 0.41 m and an initial temperature $T_i = 1\,°\mathrm{C}$ is subjected to freezing initialized at the bottom surface with a heat flux $q^* = -100\,\frac{\mathrm{w}}{\mathrm{m}^2}$, whereas all other surfaces are assumed as thermally isolated.

The obtained simulation results of the developed model is compared with the numerical results generated from the Lackner's model [20]. Both models indicate that, as soon as phase transition starts, the release of latent heat prevents the temperature from dropping. As long as the total released energy is consumed, a rapid temperature decrease is observed (Fig. 2 left). Moreover, during the freezing process, the freezing front propagates through the specimen from the bottom to the top until the entire specimen is frozen (Fig. 2 right). The comparison shows a good correlation of the numerical results for the evolution of both the temperature and the crystal saturation. Only a slight shape difference appears in the latter curve, due to use of different liquid saturation functions.

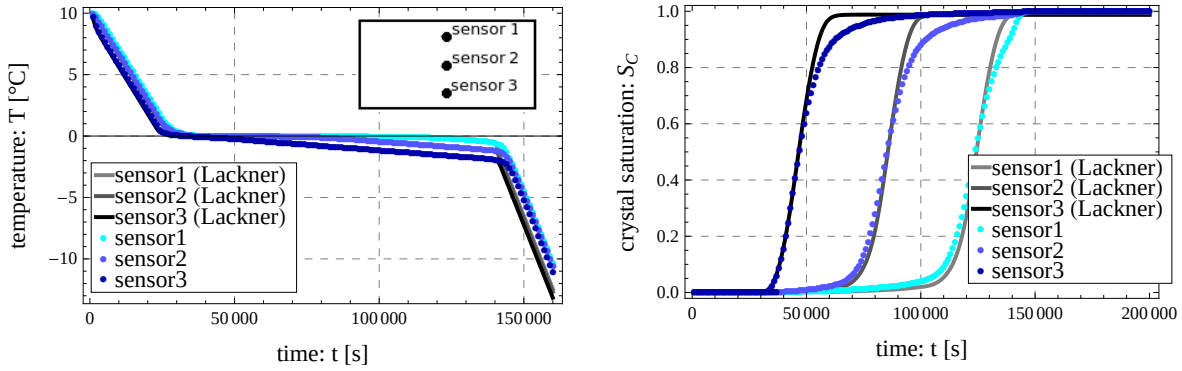

Figure 2: Model validation – phase transition with latent heat effect: Temperature (left) and ice saturation evolutions for three sensor positions

5.2 Terzaghi's consolidation problem

As a second validation example, a one dimensional consolidation test is reanalyzed numerically using the developed model. To this end, a soil layer resting on a rigid impervious base at depth $z = 1\,\mathrm{m}$, while its upper surface at $z = 0\,\mathrm{m}$ remains drained with a reference pressure $p_\mathrm{L} = 0\,\mathrm{Pa}$, is considered. For sake of simplification, gravity loading is ignored. A vertical constant load $t^* = -1000\,\frac{\mathrm{N}}{\mathrm{m}^2}$ is instantaneously applied at the upper surface.

Initially, the applied load is fully carried by the liquid water leading to an overpressurization owing to its low compressibility. Subsequently this overpressure progressively vanishes as a result of the diffusion process of the fluid towards the boundary of the soil layer which remains drained. The obtained numerical results conform perfectly with the analytical solution [1], as shown in Fig. 3. The temporal evolution of the vertical displacement of the upper surface follows an exponential characteristics, with a value of

$u = -0.09258\,\text{mm}$ at $t = 1000\,\text{s}$. This (nearly asymptotic) value is close to the analytical solution of the soil layer's drained settlement at $t = \infty$, $s_\infty = 0.09286\,\text{mm}$, where the fluid overpressure has dissipated completely.

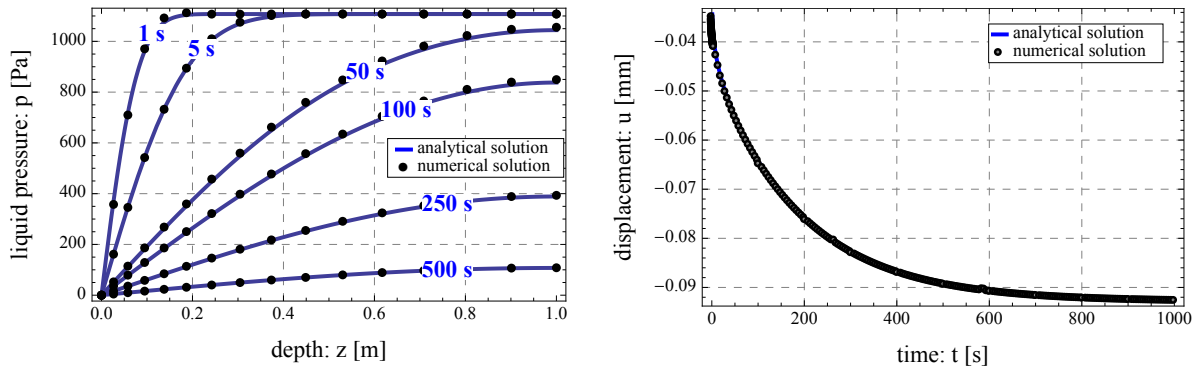

Figure 3: Model validation – consolidation test: Water pressure profiles over depth for different time instants (left); and vertical displacement evolution of upper surface (right)

5.3 Strain analysis during freezing

For the final validation of the model behavior related to the thermo-hydro-mechanical couplings, an experiment performed by Beaudoin & MacInnis [21] has been re-analyzed numerically. A cubic cement paste specimen (side length: 0.1 m), initially fully saturated by liquid water, is exposed to uniform cooling. The specimen is assumed as stress-free and undrained, i.e. no external load is applied and the total mass of water existing either in solid or liquid form remains constant.

In the absence of air voids, the porous material undergoes in general a cryo-swelling during freezing (Fig. 4). The strain analysis (Coussy [14]) shows that there are three contributions to the volumetric dilatation during freezing (Fig. 4 left). The main contribution $\varepsilon_{\Delta\rho}$ accounts for the hydraulic effect because the excess of liquid water expelled from the freezing sites, as a result of the liquid-crystal density difference, cannot escape from the sample. The other two contributions ε_{th} and $\varepsilon_{\Sigma_\text{f}}$ are consequences of the thermal contraction of the mixture and the micro-cryo-suction process caused by the difference between the liquid pressure and crystal pressure, respectively. Actually, it has been concluded that $\varepsilon_{\Sigma_\text{f}}$ is always positive even for liquids that usually contract when they solidify, and would vanish only for a zero freezing entropy [14]. This explains the dilation still observed in the experiment [3] using benzene as saturating liquid. In Fig. 4 (right) the numerical result for the overall volumetric strain during cooling is compared to analytical solution. Only small difference caused by the discretization error is observed.

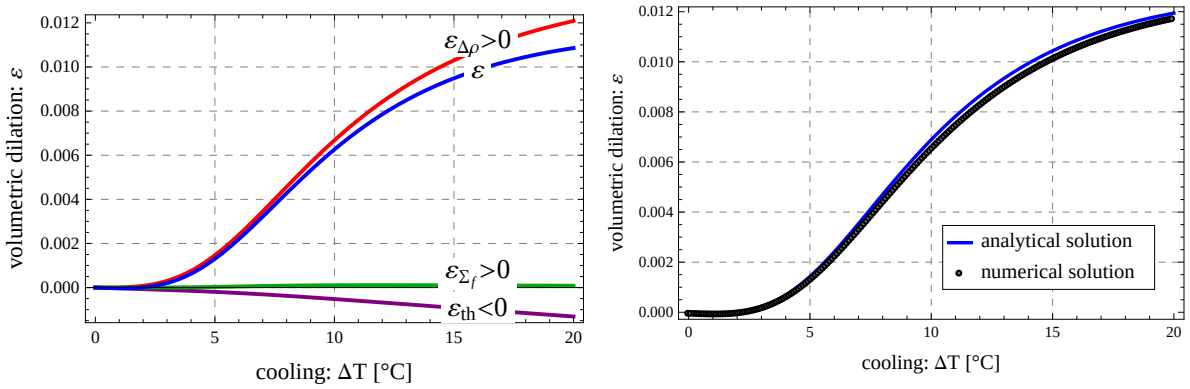

Figure 4: Model validation – thermo-hydro-mechanical couplings: Three contributions to the volumetric dilation (left) and comparison of the volumetric dilatation as obtained from the model and from analytical solution (right)

6 CONCLUSIONS AND OUTLOOK

A Finite Element model formulated within the theory of thermo-poroelasticity proposed by Coussy [1, 2] has been presented in this paper to describe the fully-coupled thermo-hydro-mechanical behavior of water-saturated soil subjected to freezing. Within the developed model, soil is treated as a three-phase porous material composed of solid skeleton, liquid water and crystal ice, where the liquid phase contains both unconfined pore water and confined water film. Instead of being specified, the latent heat associated phase transition has been incorporated via the temperature-dependent liquid saturation curve characterized by the pore size distribution. The cryo-suction mechanism, identified as the driving force for frost heave phenomenon, is impelled by the chemical potential difference existing between the supercooled pore water some distance from the freezing site and the pre-melted liquid film directly in contact with the formed crystals (cf. Eq. (2)), and has been demonstrated in the third validation example.

In the subsequent stage, a supplementary step, taking into account the formation and growth of ice lenses within the frozen fringe, is to be carried on for an integrated description of the frost heave phenomenon. Besides, a more realistic inelastic material description of the freezing soil is to be considered.

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